

Non-Weyl asymptotics for quantum graphs with general coupling conditions

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Abstract. Inspired by a recent result of Davies and Pushnitski, we study resonance asymptotics of quantum graphs with general coupling conditions at the vertices. We derive a criterion for the asymptotics to be of a non-Weyl character. We show that for balanced vertices with permutation-invariant couplings the asymptotics is non-Weyl only in case of Kirchhoff or anti-Kirchhoff conditions. For graphs without permutation numerous examples of non-Weyl behaviour can be constructed. Furthermore, we present an insight into what makes the Kirchhoff/anti-Kirchhoff coupling particular from the resonance point of view. Finally, we demonstrate a generalization to quantum graphs with unequal edge weights.

1. Introduction

Quantum graphs are objects of intense interest – we refer to [AGA08] for the history of the subject and a rich bibliography. One of their attractive features is that they are mathematically accessible while at the same time allowing an investigation of various effects uncommon in the usual quantum mechanics in Euclidean space. A very recent example was presented by a paper by one of us with Pushnitski [DP10] in which the high-energy behaviour of resonances in quantum graphs was investigated and situations were demonstrated in which the asymptotics deviates from the classical Weyl type.

To be specific, the result in [DP10] was that in some situations the graph can have asymptotically *fewer* resonances than expected. This occurs if the vertex coupling is the simplest non-trivial coupling possible, usually called Kirchhoff, and at least one graph vertex is *balanced* in the sense that it is joined to an equal number of finite internal edges and semi-infinite external edges, which we call leads. Our goal in this paper is to determine when non-Weyl resonance asymptotics occurs for quantum graphs with more general vertex couplings.

By combining some observations from a previous paper of two of us [EL10] with classical results about zeros of exponential sums [L31], we derive a criterion for a quantum graph to have a family of resonances with non-Weyl behaviour; cf. Theorem 3.3 below. We pay particular attention to quantum graphs in which the coupling condition at every vertex is invariant under all permutations of the edges joined to the vertex. Within this class we show in Theorem 4.3 that there are only two cases yielding non-Weyl asymptotics, the mentioned result of [DP10] being one of them. On the other hand, if one abandons the permutation symmetry one can produce numerous examples of graphs with such behaviour, even if none of their vertices is balanced. We explain how that happens and illustrate the result with a simple example.

We also present considerations that help to explain why the Kirchhoff conditions (and their counterpart) are so particular from the resonance point of view. First we discuss the example of a loop with two leads attached at the same point through a δ -coupling; we show that “one half” of the resonances escape to infinity as one approaches the Kirchhoff situation. Then we add a more general discussion showing, in rough terms, that a balanced vertex with Kirchhoff conditions allows for a partial decoupling which effectively diminishes the “size” of the graph which enters the asymptotics.

Finally, we discuss a class of more general graphs, whose edges have weights, in general unequal ones. In Theorem 8.3 we show that the results about non-Weyl resonance asymptotics can be extended to such systems provided the notion of a balanced vertex is modified: the issue is whether a certain linear combination of the weights vanishes at any vertex.

2. Preliminaries

We start by recalling a few notions about quantum graphs and, in particular, some concepts introduced in [EL10] and [DP10]. Consider a metric graph Γ consisting of a set of vertices \mathcal{X}_j , N internal edges with lengths l_j , $j = 1, \dots, N$, and M external semi-infinite edges. We equip it with the Hamiltonian acting on each edge as $-\mathrm{d}^2/\mathrm{d}x^2$ with appropriate coupling conditions at the vertices: the domain of the operator consists of all functions from $W^{2,2}(\Gamma)$ which satisfy

$$(U_j - I)\Psi_j + i(U_j + I)\Psi'_j = 0, \quad (1)$$

at the vertices of the graph, where U_j is a unitary $\deg \mathcal{X}_j \times \deg \mathcal{X}_j$ matrix, I stands for the unit matrix and Ψ_j and Ψ'_j are vectors of the values and the outward derivatives of

the relevant functions at the given vertex, respectively. The condition (1) is the standard unique version[‡] of the general coupling description [KS99], which was first proposed in [Ha00, KS00][§] and was derived for graphs by a straightforward method in [CE04].

Following [EL10], each graph with finitely many edges can be equivalently treated as a one-vertex-graph with the coupling given by a single “large” unitary matrix U ; the leads stem from the single vertex and all the internal edges begin and end at it. The topology of the original graph is encoded, of course, in the matrix U ; more explicitly, the condition $(U - I)\Psi + i(U + I)\Psi' = 0$ does not couple a pair of edges if they do not have any end in common.

The entities of interest are resonances of the described operator, which we will denote by H_U . They are conventionally defined as poles of the analytic continuation of $(H_U - I)^{-1}$, and they coincide with the poles of the on-shell scattering matrix on the graph Γ . It was shown in [EL10] that the resonance positions are determined by the condition

$$F(k) := \det [(U - I) C_1(k) + ik(U + I) C_2(k)] = 0, \quad (2)$$

where $C_1(k), C_2(k)$ are $(2N + M) \times (2N + M)$ matrices of the form

$$C_j(k) = \text{diag} (C_j^{(1)}(k), C_j^{(2)}(k), \dots, C_j^{(N)}(k), i^{j-1} I_{M \times M}), \quad j = 1, 2,$$

where the first $2N$ blocks are given by

$$C_1^{(j)}(k) = \begin{pmatrix} 0 & 1 \\ \sin kl_j & \cos kl_j \end{pmatrix}, \quad C_2^{(j)}(k) = \begin{pmatrix} 1 & 0 \\ -\cos kl_j & \sin kl_j \end{pmatrix},$$

respectively, and $I_{M \times M}$ is the $M \times M$ unit matrix. There is an important convention to make here. Usually one associates resonances with resolvent poles in the lower complex halfplane while those on the real axis are *eigenvalues*, typically embedded in the continuous spectrum. As in [DP10], however, the latter will be also *regarded as resonances* in this paper.

It was also shown in [EL10] that the problem can be reformulated as an investigation of the compact “internal” graph, the influence of the leads being taken into account by replacing the coupling at the “external” vertices to which the leads are attached by an effective, energy-dependent one. In particular, the resonance condition (2) can be then rewritten as

$$\det [(\tilde{U}(k) - I) \tilde{C}_1(k) + ik(\tilde{U}(k) + I) \tilde{C}_2(k)] = 0,$$

where the $2N \times 2N$ matrices $\tilde{C}_i(k)$, $i = 1, 2$, contain only the parts of $C_i(k)$ corresponding to the internal edges,

$$\tilde{C}_i(k) = \text{diag} (C_i^{(1)}(k), C_i^{(2)}(k), \dots, C_i^{(N)}(k))$$

and the unitary matrix U is replaced by the effective $2N \times 2N$ coupling matrix

$$\tilde{U}(k) := U_1 - (1 - k)U_2[(1 - k)U_4 - (k + 1)I]^{-1}U_3, \quad (3)$$

[‡] For alternative descriptions of vertex couplings see [Ku04] and [CET10].

[§] Note that the condition was already known in the general theory of boundary value problems [GG91].

where U_i refer to the block decomposition $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$ related to grouping of the internal and external edges, respectively.

As in [DP10], an external vertex of the graph Γ is called *balanced* if it connects the same number of internal and external edges, otherwise we say it is *unbalanced*.

3. The main result

Since we are interested in the high-energy asymptotics of the resonances, it is convenient to rewrite the condition (2) in terms of the exponentials e^{ikl_j} and e^{-ikl_j} . For brevity, we denote $e_j^\pm := e^{\pm ikl_j}$ and

$$e^\pm := \prod_{j=1}^N e_j^\pm = e^{\pm ikV}$$

where $V = \sum_{j=1}^n l_j$ is the size of the finite part of the graph. The condition (2) then becomes

$$\begin{aligned} F(k) := & \det \left\{ \frac{1}{2}[(U-I) + k(U+I)]E_1(k) + \frac{1}{2}[(U-I) - k(U+I)]E_2(k) \right. \\ & + k(U+I)E_3 + (U-I)E_4 \\ & \left. + [(U-I) - k(U+I)] \operatorname{diag}(0, \dots, 0, I_{M \times M}) \right\} \\ & = 0, \end{aligned} \tag{4}$$

where $E_i(k) = \operatorname{diag}(E_i^{(1)}, E_i^{(2)}, \dots, E_i^{(N)}, 0, \dots, 0)$, $i = 1, 2, 3, 4$, consists of N nontrivial 2×2 blocks

$$E_1^{(j)} = \begin{pmatrix} 0 & 0 \\ -ie_j^+ & e_j^+ \end{pmatrix}, \quad E_2^{(j)} = \begin{pmatrix} 0 & 0 \\ ie_j^- & e_j^- \end{pmatrix}, \quad E_3^{(j)} = \begin{pmatrix} i & 0 \\ 0 & 0 \end{pmatrix}, \quad E_4^{(j)} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

and a trivial $M \times M$ part.

The *counting function* $N(R, F)$ of any entire function $F(k)$ is defined by

$$N(R, F) = \#\{k : F(k) = 0 \text{ and } |k| < R\}, \tag{5}$$

where the algebraic multiplicities of the zeros are taken into account. The functions $F(k)$ that arise in the present paper are more general than those discussed in [DP10] and the asymptotics of their zeros is controlled by the following classical theorem.

Theorem 3.1. *Let $F(k) = \sum_{r=0}^n k^{\nu_r} a_r(k) e^{ik\sigma_r}$, where $\nu_r \in \mathbb{R}$, $a_r(k)$ are rational functions of the complex variable k with complex coefficients that do not vanish identically, and $\sigma_r \in \mathbb{R}$, $\sigma_0 < \sigma_1 < \dots < \sigma_n$. Suppose also that ν_r are chosen so that $\lim_{k \rightarrow \infty} a_r(k) = \alpha_r$ is finite and non-zero for all r . There exists a compact set $\Omega \subset \mathbb{C}$, real numbers m_r and positive K_r , $r = 1, \dots, n$, such that the zeros of $F(k)$ outside Ω lie in one of n logarithmic strips, each one bounded between the curves $-\operatorname{Im} k + m_r \log |k| = \pm K_r$. The counting function behaves in the limit $R \rightarrow \infty$ as*

$$N(R, F) = \frac{\sigma_n - \sigma_0}{\pi} R + \mathcal{O}(1).$$

Proof. The claim follows, e.g., from Theorem 6 in [L31]. First of all, we note that there are finitely many zeros (counting multiplicities) in Ω which naturally do not influence the asymptotics. Secondly, our $F(k)$ belongs to the class $\sum_{r=0}^n k^{\nu_r}(\alpha_r + o(1))e^{ik\sigma_r}$ treated in Section 7 of [L31]. The localization of zeros described in the theorem follows directly from the conclusions there.

The number of zeros in the circle with centre 0 and diameter R can be estimated from above by the number of zeros satisfying $|\operatorname{Re} k| \leq R$ and from below by the number of zeros satisfying $|\operatorname{Re} k| \leq \sqrt{R^2 - (K + m \log R)^2}$ with $K := \max_{1 \leq r \leq n} K_r$ and $m := \max_{1 \leq r \leq n} |m_r|$. Since $R - \sqrt{R^2 - (K + m \log R)^2} \rightarrow 0$ as $R \rightarrow \infty$, both pairs of lines asymptotically approach each other. The number of zeros in the j -th logarithmic strip between two lines parallel to the imaginary axis is given by relation (7) in [L31] with c_n being replaced by the distance of corresponding σ_j 's, hence the asymptotic behaviour of the counting function is given by the above relation. \square

To apply this theorem we have to determine the coefficients of e^\pm in the resonance condition (4). To this aim it is more convenient to use the formulation with a compact graph and energy-dependent matrices, since the last term in (4) then disappears and the relation thus becomes

$$\begin{aligned} F(k) &:= \det \left\{ \frac{1}{2}[(\tilde{U}(k) - I) + k(\tilde{U}(k) + I)]\tilde{E}_1(k) \right. \\ &\quad + \frac{1}{2}[(\tilde{U}(k) - I) - k(\tilde{U}(k) + I)]\tilde{E}_2(k) \\ &\quad \left. + k(\tilde{U}(k) + I)\tilde{E}_3 + (\tilde{U}(k) - I)\tilde{E}_4 \right\} \\ &= 0, \end{aligned} \tag{6}$$

where \tilde{E}_j (the first two of them being energy-dependent) are the nontrivial $2N \times 2N$ parts of the matrices E_j and I denotes the $2N \times 2N$ unit matrix.

Lemma 3.2. *The coefficient of e^\pm in (6) is $\left(\frac{i}{2}\right)^N \det[(\tilde{U}(k) - I) \pm k(\tilde{U}(k) + I)]$.*

Proof. Let us prove the claim for the coefficient of e^+ . First of all, note that one does not need to consider the term involving $E_2(k)$, since all the entries of E_2 diminish the imaginary part of the argument of the exponential. Furthermore, bearing in mind that the determinant is not changed by a similarity transformation, we diagonalize the matrix $E_1(k)$ using the block diagonal matrix V consisting of 2×2 blocks $\begin{pmatrix} 0 & -i \\ 1 & 1 \end{pmatrix}$ and look for the coefficient of e^+ in the determinant

$$\begin{aligned} &\det \left\{ \frac{1}{2}V^{-1}[(\tilde{U}(k) - I) + k(\tilde{U}(k) + I)]V\tilde{E}_{1V} \right. \\ &\quad \left. + kV^{-1}(\tilde{U}(k) + I)V\tilde{E}_{3V} + V^{-1}(\tilde{U}(k) - I)V\tilde{E}_{4V} \right\}, \end{aligned}$$

where the transformed matrices $\tilde{E}_{iV} = V^{-1}\tilde{E}_iV$ are still block diagonal with the blocks

$$\tilde{E}_{1V}^{(j)} = \begin{pmatrix} e_j^+ & 0 \\ 0 & 0 \end{pmatrix}, \quad \tilde{E}_{3V}^{(j)} = \begin{pmatrix} 0 & -i \\ 0 & i \end{pmatrix}, \quad \tilde{E}_{4V}^{(j)} = \begin{pmatrix} -i & -i \\ i & i \end{pmatrix}.$$

In order to obtain the maximum possible imaginary part of the exponent one has to choose the odd column contributions to the determinant only from the term containing \tilde{E}_{1V} . Hence the odd columns of $\tilde{E}_{4V}^{(j)}$ do not influence the coefficient of e^+ and our task simplifies to determining the coefficient of e^+ in

$$\det \{[(\tilde{U}(k) - I) + k(\tilde{U}(k) + I)](\frac{1}{2}\tilde{E}_{1V} + \tilde{E}_{3V})\} = \frac{i^N}{2^N} \det[(\tilde{U}(k) - I) + k(\tilde{U}(k) + I)] e^+.$$

The argument for e^- is similar, one need not consider now the term with \tilde{E}_{1V} and chooses V that diagonalizes \tilde{E}_{2V} . \square

Combining Theorem 3.1 with the previous lemma we arrive at the conclusion which is useful in determining whether resonances of a given quantum graph Hamiltonian have Weyl asymptotics or not.

Theorem 3.3. *Let us assume a quantum graph (Γ, H_U) corresponding to Γ with finitely many edges and the coupling at vertices \mathcal{X}_j given by unitary matrices U_j . The asymptotics of the resonance counting function as $R \rightarrow \infty$ is of the form*

$$N(R, F) = \frac{2W}{\pi} R + \mathcal{O}(1),$$

where we call W the effective size of the graph. One always has

$$0 \leq W \leq V := \sum_{j=1}^N l_j.$$

Moreover $W < V$ (in other words, the graph is non-Weyl in the terminology of [DP10]) if and only if there exists a vertex where the corresponding energy-dependent coupling matrix $\tilde{U}_j(k)$ has an eigenvalue $(1 - k)/(1 + k)$ or $(1 + k)/(1 - k)$ for all k .

Proof. It follows from Lemma 3.2 and Theorem 3.1 that a graph is non-Weyl iff the “overall-vertex” coupling matrix $\tilde{U}(k)$ has eigenvalue $(1 - k)/(1 + k)$ or $(1 + k)/(1 - k)$.

Note that one need not worry about the limiting assumptions in the theorem; if $a_0(k)$ or $a_n(k)$ are $\mathcal{O}(k^{-m})$, one can replace $F(k)$ by $\tilde{F}(k) := k^m F(k)$, which adds only a resonance of finite multiplicity at $k = 0$, and apply the argument to $\tilde{F}(k)$. In general Γ is a multivertex graph, of course, but the “overall” unitary coupling matrix U is block diagonal, hence $\tilde{U}(k)$ also decouples into effective coupling matrices for particular vertices and their eigenvalues can be computed separately. \square

4. Permutation-symmetric coupling

In this section we apply the above results to graphs whose coupling at every vertex is invariant with respect to permutations of the edges at the vertex. It is easy to see that the coupling is described by matrices of the form $U_j = a_j J + b_j I$, where a_j, b_j are complex numbers satisfying $|b_j| = 1$ and $|b_j + a_j \deg \mathcal{X}_j| = 1$; the symbol J denotes the square matrix all of whose entries equal to one and I stands for the unit matrix.

The class of coupling conditions with permutation symmetry includes two most important particular cases — the δ -conditions with $U_j = \frac{2}{d_j + i\alpha_j}J - I$, where d_j is the number of edges emanating from the vertex \mathcal{X}_j and $\alpha_j \in \mathbb{R}$ is the coupling strength, and the δ'_s -conditions corresponding to $U_j = -\frac{2}{d_j - i\beta_j}J + I$ with $\beta_j \in \mathbb{R}$. The particular case $\alpha_j = 0$ of the δ -coupling is the so-called Kirchhoff condition — *free* would be a better name — which was discussed in [DP10].

Let us consider a vertex which connects p internal and q external edges. For simplicity, we omit the subscript j labeling the vertex. On the other hand, to avoid confusion we mark the size of the matrices J and I . As a preliminary, we state the following lemma without its proof, which is straightforward.

Lemma 4.1. *The matrix $U = aJ_{n \times n} + bI_{n \times n}$ has $n - 1$ eigenvalues b and one eigenvalue $na + b$. Its inverse is $U^{-1} = -\frac{a}{b(an+b)}J_{n \times n} + \frac{1}{b}I_{n \times n}$.*

Next we give an explicit expression for the effective coupling.

Lemma 4.2. *Suppose that p internal and q external edges are connected by means of the coupling given by $U = aJ_{(p+q) \times (p+q)} + bI_{(p+q) \times (p+q)}$. Then the corresponding energy-dependent coupling matrix is*

$$\tilde{U}(k) = \frac{ab(1-k) - a(1+k)}{(aq+b)(1-k) - (k+1)}J_{p \times p} + bI_{p \times p}.$$

Proof. The matrix $\tilde{U}(k)$ is defined by the expression (3), where $U_1 = aJ_{p \times p} + bI_{p \times p}$, $U_4 = aJ_{q \times q} + bI_{q \times q}$, and U_2 and U_3 are rectangular $p \times q$ and $q \times p$ matrices, respectively, with all the entries equal to a . The needed inverse is easily computed with the help of the previous lemma. \square

As the main result of this section, we show that in the whole two-parameter class of permutation-symmetric coupling conditions there are only two cases which exhibit non-Weyl asymptotics. Specifically, a quantum graph with δ or δ'_s -conditions can be non-Weyl only if the corresponding coupling strength is zero.

Theorem 4.3. *Let (Γ, H_U) be a quantum graph with permutation-symmetric coupling conditions at the vertices, $U_j = a_jJ + b_jI$. Then it has non-Weyl asymptotics if and only if at least one of its vertices is balanced in the sense that $p = q$, and the coupling at this vertex is either*

$$(a) \quad f_m = f_n, \quad \forall m, n \leq 2p, \quad \sum_{m=1}^{2p} f'_m = 0, \quad \text{i.e. } U = \frac{1}{p}J_{2p \times 2p} - I_{2p \times 2p},$$

or

$$(b) \quad f'_m = f'_n, \quad \forall m, n \leq 2p, \quad \sum_{m=1}^{2p} f_j = 0, \quad \text{i.e. } U = -\frac{1}{p}J_{2p \times 2p} + I_{2p \times 2p}.$$

Proof. Using Lemmata 4.1 and 4.2 together with Theorem 3.3 we have to determine the values of a , b , p and q for which the matrix $\tilde{U}(k)$ has an eigenvalue $(1 \pm k)/(1 \mp k)$. Since $|b| = 1$, the only possibility is that the relation

$$ap \frac{b(1-k) - (1+k)}{(aq+b)(1-k) - (k+1)} + b = \frac{1 \pm k}{1 \mp k}.$$

holds for all k . One of the cases yields

$$[a(p+q)+b]b(1-k) - (ap+aq+2b)(1+k) = -\frac{(1+k)^2}{1-k},$$

which cannot be satisfied for any value of the parameters a, b, p and q . The other case yields

$$\{[a(p+q)+b]b+1\}(1-k) - (1+k)(ap+b) = (aq+b)\frac{(1-k)^2}{1+k}.$$

Since this has to be true for all k we have

$$\begin{aligned} ap+b=0, \quad aq+b=0 &\Rightarrow p=q, \\ [a(p+q)+b]b+1=0 &\Rightarrow (ap)^2=1, \end{aligned}$$

and consequently, the graph is non-Weyl iff $U = \pm \frac{1}{p} J_{p \times p} \mp I_{p \times p}$. \square

5. Unbalanced non-Weyl graphs

We next describe a method of constructing unbalanced graphs with non-Weyl asymptotic behaviour. For simplicity, we only treat a simple example; an extension to more complicated graphs is straightforward.

The trick we use is based on replacing the coupling matrix U by $W^{-1}UW$, where W is a block diagonal matrix of the form

$$W = \begin{pmatrix} e^{i\varphi} I_{p \times p} & 0 \\ 0 & W_4 \end{pmatrix}.$$

and W_4 is a unitary $q \times q$ matrix.

Lemma 5.1. *The family of resonances of H_U does not change if the original coupling matrix U is replaced by $W^{-1}UW$.*

Proof. If $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$ then $W^{-1}UW = U_W = \begin{pmatrix} U_1 & U_2 W_4 e^{-i\varphi} \\ W_4^{-1} U_3 e^{i\varphi} & W_4^{-1} U_4 W_4 \end{pmatrix}$. The effective energy-dependent coupling matrix $\tilde{U}_W(k)$ corresponding to $W^{-1}UW$ as in (3) is given by

$$\begin{aligned} \tilde{U}_W(k) &= U_1 - (1-k)U_2 e^{-i\varphi} W_4 \{W_4^{-1}[(1-k)U_4 - (k+1)I]W_4\}^{-1} W_4^{-1} U_3 e^{i\varphi} \\ &= \tilde{U}(k). \end{aligned}$$

In other words, since W commutes with $C_i(k)$ the resonance condition (2) is not affected by the similarity transformation. \square

Our next example uses this transformation to construct unbalanced graphs with non-Weyl asymptotics.

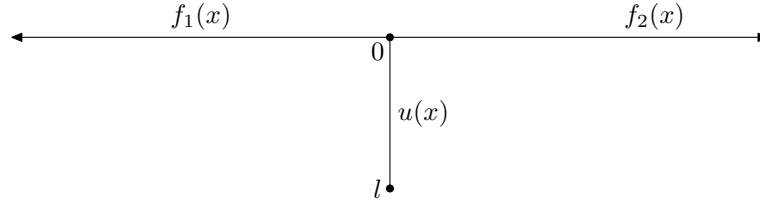


Figure 1. Graph with two leads and one internal edge

Example 5.2. Consider a quantum particle with the Hamiltonian acting as $-\mathrm{d}^2/\mathrm{d}x^2$ on the graph Γ consisting of two half-lines and one internal edge of length l , as sketched in Figure 1, studied for the first time in [EŠ94]. The domain of the Hamiltonian consists of functions from $W^{2,2}(\Gamma)$ which satisfy the coupling conditions

$$\begin{aligned} 0 &= (U - I) (u(0), f_1(0), f_2(0))^T + i(U + I) (u'(0), f_1'(0), f_2'(0))^T, \\ 0 &= u(l) + cu'(l), \end{aligned}$$

where $f_i(x)$ are functions on the half-lines and $u(x)$ refers to the internal edge.

We start from the Robin condition $u(l) + cu'(l) = 0$ at the free end of the internal edge and the coupling matrix $U_0 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & e^{i\psi} \end{pmatrix}$.

One may alternatively represent the graph as two disjoint half-lines; one has a Robin condition parametrized by ψ at its endpoint, while the other is obtained by joining a half-line to the original internal edge by means of a free (Kirchhoff) coupling. Using the original specification, the graph has non-Weyl asymptotics by [DP10] or Theorem 3.3. Indeed it cannot have more than two resonances.

We now perform a transformation replacing U by $U_W = W^{-1}UW$ with

$$W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & re^{i\varphi_1} & \sqrt{1-r^2}e^{i\varphi_2} \\ 0 & \sqrt{1-r^2}e^{i\varphi_3} & -re^{i(\varphi_2+\varphi_3-\varphi_1)} \end{pmatrix}$$

and obtain for every fixed value of ψ and c a three-parameter family of coupling conditions described by the unitary matrix

$$U = \begin{pmatrix} 0 & re^{i\varphi_1} & \sqrt{1-r^2}e^{i\varphi_2} \\ re^{-i\varphi_1} & (1-r^2)e^{i\psi} & -r\sqrt{1-r^2}e^{-i(-\psi+\varphi_1-\varphi_2)} \\ \sqrt{1-r^2}e^{-i\varphi_2} & -r\sqrt{1-r^2}e^{i(\psi+\varphi_1-\varphi_2)} & r^2e^{i\psi} \end{pmatrix},$$

each of which has the same resonances as U_0 by Lemma 5.1. The associated quantum graphs have only two resonances and are therefore of non-Weyl type.

Remark 5.3. Choosing Dirichlet conditions both at the end of the separated half-line, $\psi = \pi$, and at the remote end of the internal edge, $c = 0$, one obtains a family of

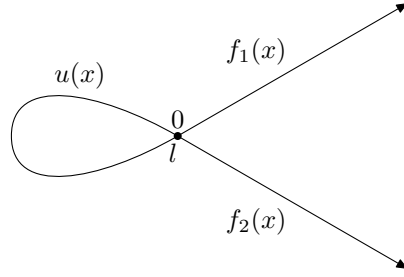


Figure 2. A loop graph with two leads

Hamiltonians which have no resonances at all. This class contains the example pointed out in [EŠ94]: the choice $\varphi_1 = \varphi_2 = 0$ and $r = 1/\sqrt{2}$ corresponds to the coupling

$$f_1(0) = f_2(0), \quad u(0) = \sqrt{2}f_1(0), \quad f_1'(0) - f_2'(0) = -\sqrt{2}u'(0),$$

or in terms of [EŠ94] $b = \sqrt{2}, c = d = 0$. Similarly, the second possibility indicated in [EŠ94], i.e. $b = -\sqrt{2}, c = d = 0$, can be obtained by choosing $\varphi_1 = \varphi_2 = \pi$ and $r = 1/\sqrt{2}$. Notice also that the absence of resonances in this case is easily understood if one regards the graph in question as a tree with the root at the remote end of the internal edge and employs a unitary equivalence proposed first by Solomyak – see, e.g., [SS02].

6. A loop with two leads

We have seen that the resonance asymptotics can be changed by varying the coupling parameters of the model. This motivates us to analyze another simple example. The graph Γ , as sketched on Figure 2, now consists of a loop of length l and two half-lines attached to it at one point. The Hilbert space is $L^2(0, l) \oplus L^2(\mathbb{R}_+) \oplus L^2(\mathbb{R}_+)$ with its elements written as $(u(x), f_1(x), f_2(x))^T$. The Hamiltonian acts as $-d^2/dx^2$ and its domain will consist of functions from $W^{2,2}(\Gamma)$ satisfying the conditions

$$\begin{aligned} u(0) &= f_1(0), \quad u(l) = f_2(0), \\ \alpha u(0) &= u'(0) + f_1'(0) + \beta(-u'(l) + f_2'(0)), \\ \alpha u(l) &= \beta(u'(0) + f_1'(0)) - u'(l) + f_2'(0) \end{aligned} \tag{7}$$

with real parameters α and β . The choice $\beta = 1$ corresponds to the “overall” δ -condition of strength α , while $\beta = 0$ decouples two “inner-outer” pairs of meeting edges and one obtains a line with two δ -interactions at the distance l .

In this particular case the resonance condition (2) can be written as

$$16 \frac{-\alpha^2 \sin kl + 2k\alpha(\beta + i \sin kl - \cos kl) - 2k^2(\sin kl + i \cos kl)(\beta^2 - 1)}{4(\beta^2 - 1) + \alpha(\alpha - 4i)} = 0 \tag{8}$$

or in terms of e^\pm introduced in Section 3

$$8 \frac{i\alpha^2 e^+ + 4k\alpha\beta - i[\alpha(\alpha - 4ik) + 4k^2(\beta^2 - 1)] e^-}{4(\beta^2 - 1) + \alpha(\alpha - 4i)} = 0.$$

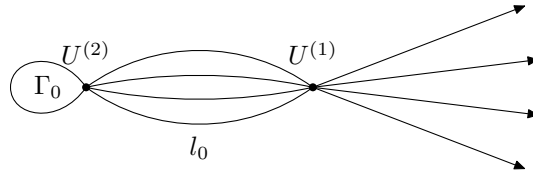


Figure 3. Graph with a balanced vertex considered in Proposition 7.1

We see that the coefficient of e^+ vanishes iff $\alpha = 0$, the second term vanishes for $\beta = 0$ or if $|\beta| \neq 1$ and $\alpha = 0$, while the polynomial multiplying e^- does not vanish for any combination of α and β .

In other words, the graph has non-Weyl asymptotics iff $\alpha = 0$. If, in addition, $|\beta| \neq 1$, then all resonances are confined to some circle, i.e. the graph has zero “effective size”. The only exceptional cases are the Kirchhoff condition, $\beta = 1$ and $\alpha = 0$, and its counterpart condition $\beta = -1$ and $\alpha = 0$, for which one half of the resonances is asymptotically preserved, in other words, the effective size of the graph is $l/2$.

Let us look at the δ -condition, $\beta = 1$, in more detail in order to illustrate the disappearance of half of the resonances when the coupling strength vanishes. The resonance equation (8) becomes

$$\frac{-\alpha \sin kl + 2k(1 + i \sin kl - \cos kl)}{\alpha - 4i} = 0.$$

A simple calculation shows that the graph Hamiltonian has a sequence of embedded eigenvalues, $k = 2n\pi/l$ with $n \in \mathbb{Z}$, and a family of resonances given by solutions to $e^{ikl} = -1 + \frac{4ik}{\alpha}$. The former do not depend on α , while the latter behave for small α like

$$\operatorname{Im} k = -\frac{1}{l} \log \frac{1}{\alpha} + \mathcal{O}(1), \quad \operatorname{Re} k = n\pi + \mathcal{O}(\alpha),$$

therefore all the (true) resonances escape to infinity as $\alpha \rightarrow 0$.

7. What can cause non-Weyl asymptotics

We have seen that once we allow for general (self-adjoint) coupling at graph vertices the non-Weyl asymptotic behaviour of resonances may occur easily. On the other hand, the argument was based on properties of graphs with edge-permutation symmetries. The most interesting question posed by the result of [DP10] is thus what makes balanced graphs with Kirchhoff coupling — or its “anti-Kirchhoff” counterpart of Theorem 4.3 — particular among such graphs.

7.1. Kirchhoff “size reduction”

To answer this question, consider the graph Γ sketched in Figure 3. It contains a balanced vertex \mathcal{X}_1 which connects p internal edges of the same length l_0 and p external

edges with the coupling (1) given by a unitary matrix $U^{(1)} = aJ_{2p \times 2p} + bI_{2p \times 2p}$. The coupling of the other internal edge ends to the rest of the graph, denoted as Γ_0 , is described by a $q \times q$ matrix $U^{(2)}$, where $q \geq p$; needless to say such a matrix can hide different topologies of this part of the graph.

Notice first that switching off the coupling between the “inner-outer” pairs of edges may lead to different results. If, for instance, the coupling given by $U^{(1)}$ is Kirchhoff and the decoupling leads to Kirchhoff at each pair, the size of the graph is diminished by pl_0 . If on the other hand, we start from a nontrivial δ -coupling and the decoupling leads to a δ -interaction on each edge pair, the graph size remains preserved. The question is now whether the return to the “full” coupling in the former case can restore the size.

To demonstrate that this is not the case and that the effective size of the graph is smaller in the case of Kirchhoff and “anti-Kirchhoff” condition at the balanced vertex one can employ a trick similar to the one used in Lemma 5.1.

Proposition 7.1. *Let Γ be the described graph with the coupling given by arbitrary $U^{(1)}$ and $U^{(2)}$. Let V be an arbitrary unitary $p \times p$ matrix, $V^{(1)} := \text{diag}(V, V)$ and $V^{(2)} := \text{diag}(I_{(q-p) \times (q-p)}, V)$ be $2p \times 2p$ and $q \times q$ block diagonal matrices, respectively. Then H on Γ is unitarily equivalent to the Hamiltonian H_V on topologically the same graph with the coupling given by the matrices $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ and $[V^{(2)}]^{-1}U^{(2)}V^{(2)}$.*

Proof. Let u be an element of the domain of H , u_1, \dots, u_p its restrictions to the internal edges emanating from \mathcal{X}_1 , f_1, \dots, f_p its restrictions to the external edges emanating from \mathcal{X}_1 and u_0 its restriction to the rest of the graph Γ_0 . Then the map

$$\begin{aligned} (u_1, \dots, u_p)^T &\mapsto (v_1, \dots, v_p)^T = V^{-1}(u_1, \dots, u_p)^T \\ (f_1, \dots, f_p)^T &\mapsto (g_1, \dots, g_p)^T = V^{-1}(f_1, \dots, f_p)^T \\ u_0(x) &\mapsto v_0(x) = u_0(x) \end{aligned}$$

is a bijection of the domain of H onto the domain of H_V . One can easily check that the equation (1) with the coupling matrices $U^{(1)}$ and $U^{(2)}$ transforms into that with the coupling matrices $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ and $[V^{(2)}]^{-1}U^{(2)}V^{(2)}$. \square

Remark 7.2. The assumption that the internal edges emanating from \mathcal{X}_1 have the same length is made for convenience only. If it is not satisfied one can still use the above result. To this aim it is sufficient to denote the length of the shortest of these edges by l_0 and to introduce additional vertices with Kirchhoff condition at the remaining edges at the distance l_0 from \mathcal{X}_1 . Similarly, if there is a loop at \mathcal{X}_1 , one can introduce a vertex with Kirchhoff condition in the middle of it.

The application of the above result to symmetric couplings, $U^{(1)} = aJ_{2p \times 2p} + bI_{2p \times 2p}$ at \mathcal{X}_1 , is straightforward. It is enough to choose the columns of V as an orthonormal set of eigenvectors of the corresponding $p \times p$ block $aJ_{p \times p} + bI_{p \times p}$, the first one of them being $\frac{1}{\sqrt{p}}(1, 1, \dots, 1)^T$. The transformed matrix $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ decouples then into blocks connecting only the pairs (v_j, g_j) . The first one of these, corresponding to a symmetrization of all the u_j 's and f_j 's, leads to the 2×2 matrix $U_{2 \times 2} =$

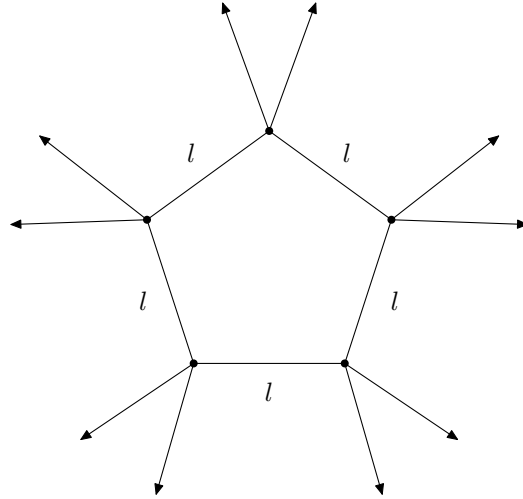


Figure 4. A polygon with pairs of leads considered in Theorem 7.3

$apJ_{2 \times 2} + bI_{2 \times 2}$, while the other lead to separation of the corresponding internal and external edges described by the Robin conditions $(b - 1)v_j(0) + i(b + 1)v'_j(0) = 0$ and $(b - 1)g_j(0) + i(b + 1)g'_j(0) = 0$ for $j = 2, \dots, p$. Notice that this resembles again the reduction of a tree graph due to Solomyak which we have mentioned in Remark 5.3.

It is easy to see that the “overall” Kirchhoff/anti-Kirchhoff condition at \mathcal{X}_1 is transformed to the “line” Kirchhoff/anti-Kirchhoff condition in the subspace of permutation-symmetric functions. Hence the size of the graph is reduced by l_0 in the Kirchhoff case. The same is true in the anti-Kirchhoff situation since these conditions on the line are trivially equivalent to Kirchhoff, in other words, to the absence of any interaction. In all the other cases the point interaction corresponding to the matrix $apJ_{2 \times 2} + bI_{2 \times 2}$ is nontrivial, and consequently, the graph size is preserved.

7.2. Calculating the effective size

Since the occurrence of non-Weyl asymptotics for a graph Γ subject to Kirchhoff boundary conditions depends on the existence of a balanced vertex, one might hope to calculate the effective size of non-Weyl graphs by using some geometrical rules that quantify the effect of each balanced vertex on the asymptotics. The following example suggests that this will not be easy. The effective sizes of the highly symmetrical graphs discussed below depend on whether a certain integer is or is not equal to 0 mod 4, and calculating the effective sizes is therefore a global rather than a local issue.

We construct a graph Γ_n for each integer $n \geq 3$ by starting with a regular n -gon, each edge of which has length ℓ . We then attach two semi-infinite leads to each vertex, so that each of the n vertices is balanced; cf. Figure 4. It follows that the effective size W_n of the graph is strictly less than the actual size $V_n = n\ell$.

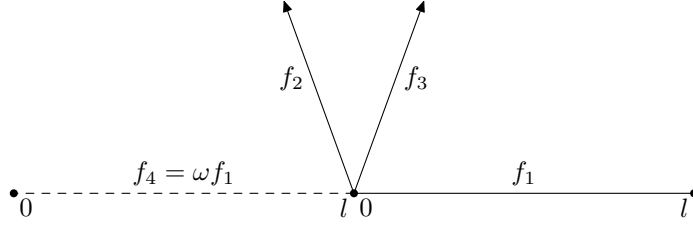


Figure 5. The four-edge graph cell considered in the proof of Theorem 7.3

Theorem 7.3. *The effective size of the graph Γ_n is given by*

$$W_n = \begin{cases} n\ell/2 & \text{if } n \not\equiv 0 \pmod{4}, \\ (n-2)\ell/2 & \text{if } n \equiv 0 \pmod{4}. \end{cases}$$

Proof. We start by constructing the Bloch/Floquet decomposition of H with respect to the cyclic rotation group \mathbb{Z}_n . Let T denote the unitary rotation operator in $L^2(\Gamma_n)$ which takes each vertex to the next vertex in the clockwise direction. We observe that $L^2(\Gamma_n)$ is the orthogonal direct sum of \mathcal{H}_ω over all complex ω satisfying $\omega^n = 1$, where

$$\mathcal{H}_\omega = \{f \in L^2(\Gamma_n) : Tf = \omega f\}.$$

Since the Hamiltonian H commutes with T it follows that the set of resonances of H is obtained as the union of the corresponding quantities for the restrictions H_ω of H to \mathcal{H}_ω . Our main task is to compute these explicitly.

Let us fix an ω satisfying $\omega^n = 1$. The resonances of H_ω can be determined by restricting attention to a cell consisting of the four edges that are attached to a chosen vertex – cf. Figure 5. A typical resonance eigenfunction f must be of the form

$$\begin{aligned} f_1(x) &= \alpha e^{ikx} + \beta e^{-ikx}, & 0 \leq x \leq \ell, \\ f_2(x) &= (\alpha + \beta) e^{ikx}, & 0 \leq x < \infty, \\ f_3(x) &= (\alpha + \beta) e^{ikx}, & 0 \leq x < \infty, \\ f_4(x) &= \omega f_1(x), & 0 \leq x \leq \ell, \end{aligned}$$

where the vertex v corresponds to the choice $x = 0$ for f_1, f_2, f_3 and to $x = \ell$ for f_4 .

The continuity condition and Kirchhoff boundary condition at v are

$$\begin{aligned} \omega \alpha e^{ik\ell} + \omega \beta e^{-ik\ell} &= \alpha + \beta, \\ \omega \alpha e^{ik\ell} - \omega \beta e^{-ik\ell} &= 2(\alpha + \beta) + \alpha - \beta. \end{aligned}$$

After evaluating the relevant 2×2 determinant one finds that one has a resonance at k if and only if

$$-2(\omega^2 + 1) + 4\omega e^{-ik\ell} = 0. \quad (9)$$

Therefore the effective size W_ω of the system of resonances of H_ω is $\ell/2$ if $\omega^2 + 1 \neq 0$ but it is 0 if $\omega^2 + 1 = 0$. Now $\omega^2 + 1 = 0$ is not soluble if $\omega^n = 1$ and $n \not\equiv 0 \pmod{4}$, but

it has two solutions if $n = 0 \bmod 4$. The statement of the theorem now follows from the observation that the effective size W_n of Γ_n is given by $W_n = \sum_{\omega^n=1} W_\omega$. \square

Note that if one puts $\omega = e^{i\theta}$ in (9) then one obtains

$$k = \frac{1}{l} \left(i \log(\cos(\theta)) + 2\pi n \right)$$

where $n \in \mathbb{Z}$ is arbitrary. From this equation it is clear that the resonances all diverge to ∞ as $\theta \rightarrow \pm\pi/2$.

8. A generalization: graphs with weighted edges

In this final section we discuss another generalization. It is useful to realize that Laplacians on metric graphs are just the simplest model for networks of quantum wires. One can, for instance, consider Sturm-Liouville operators on weighted L^2 spaces which describe thin networks of wires with different, in general varying cross sections [KZ01, EP09]. Here we will investigate another possibility which corresponds to scaling the wires longitudinally. This can have a physical interpretation; recall that the Hamiltonian on an edge is in reality $-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2}$ where m^* is the appropriate effective mass, hence joining wires of different materials we obtain such a scaling.

Consider a general graph Γ with finitely many edges, equipped now with the Hamiltonian $-c_e^2 d^2/dx^2$ on the edge e , the c_e 's being positive constants. Its domain consists of functions from $W^{2,2}(\Gamma)$ satisfying the generalized Kirchhoff coupling conditions at each vertex v , namely

$$\sum_{e:v \in e} c_e^2 f'_e(v) = 0, \quad f_{e_i}(v) = f_{e_j}(v) \quad \text{whenever } v \in e_i, e_j. \quad (10)$$

In other words, the values of the functions are continuous at each vertex and the sum of the outward derivatives weighted by c_e^2 vanishes. For the sake of simplicity we refrain from discussing the general coupling conditions.

Before turning to the general theory, we illustrate the asymptotics of weighted graphs by the following simple example.

Example 8.1. Consider again the graph consisting of one internal edge and two leads, as in Figure 1. The Hamiltonian acts now as $-c^2 d^2/dx^2$ at the internal edge and as $-\tilde{c}_j^2 d^2/dx^2$, $j = 1, 2$ at the leads. We employ the coupling conditions (10) at the junction with the wavefunctions denoted as in Figure 1, and Dirichlet condition at the free end of the internal edge,

$$f_1(0) = f_2(0) = u(0), \quad \tilde{c}_1^2 f_1(0)' + \tilde{c}_2^2 f_2(0)' + c^2 u(0)' = 0, \quad u(l) = 0.$$

Solving the Schrödinger equation explicitly for energy k^2 one gets from the coupling condition at the junction

$$c^2 \frac{k}{c} \cos \frac{kl}{c} = \tilde{c}_1^2 \frac{ik}{\tilde{c}_1} \sin \frac{kl}{c} + \tilde{c}_2^2 \frac{ik}{\tilde{c}_2} \sin \frac{kl}{c}$$

which leads to

$$(c - \tilde{c}_1 - \tilde{c}_2) e^{ikl/c} + (c + \tilde{c}_1 + \tilde{c}_2) e^{-ikl/c} = 0.$$

Consequently, this graph is non-Weyl iff $c = \tilde{c}_1 + \tilde{c}_2$, which can be regarded as a generalization of the Kirchhoff coupling conditions. The topology of the graph, namely the fact that the single vertex is unbalanced, has no significance in this example.

Our general asymptotic theorem for weighted graphs may be proved by two methods. The calculations in [DP10] may be modified line by line to include the relevant weights on each edge. We describe here an alternative approach which is simpler in the light of the analysis in this paper. It depends on the fact that the weighted graph can be transformed into a graph with all the weights equal to one by changing the lengths of the edges. This leads to boundary value conditions at each vertex of a type that were not considered in [DP10]. The interest of our main result, Theorem 8.3, is that it leads to a new insight into the nature of the ‘balanced vertex’ condition.

Lemma 8.2. *Let Γ be a weighted graph with the lengths of the internal edges l_j , their weights c_j^2 , and the weights of the external edges \tilde{c}_j^2 , both entering the coupling conditions (10). Then the corresponding weighted Hamiltonian on Γ is unitarily equivalent to the non-weighted operator, i.e. the Laplacian, on the graph Γ' with the lengths of the edges l_j/c_j and the coupling*

$$\sum_{e:v \in e} \sqrt{c_e} g'_e(v) = 0, \quad \frac{1}{\sqrt{c_{e_i}}} g_{e_i}(v) = \frac{1}{\sqrt{c_{e_j}}} g_{e_j}(v) \quad \text{whenever } v \in e_i, e_j$$

with c_e being the common symbol for both the c_j and \tilde{c}_j .

Proof. The transformation of the wavefunction on each internal and external edge $f_j(x) \mapsto g_j(y) = \sqrt{c_j} f_j(c_j y)$, $y \in (0, l_j/c_j)$ leads to $g_j(0) = \sqrt{c_j} f_j(0)$ and $g'_j(0) = \sqrt{c_j^3} f'_j(0)$, and similarly for the external edges. Substituting these expressions into (10) we arrive at the indicated coupling for the g_j ’s. \square

Notice that in view of the previous lemma the natural definition of the size of the weighted graph is $V = \sum_j l_j/c_j$ where the sum runs over all the internal edges. Using the lemma in combination with the results of Sec. 7.1 one can prove the following.

Theorem 8.3. *Let Γ be a weighted graph with the weights described above and the coupling conditions (10). Then the Hamiltonian has non-Weyl asymptotics iff for at least one of its vertices v the relation*

$$\sum_{e:v \in e} c_e = \sum_{\tilde{e}:v \in \tilde{e}} c_{\tilde{e}}$$

holds, where e and \tilde{e} stand for the internal and external edges emanating from the vertex v , respectively.

Proof. With the help of the transformation from Lemma 8.2 one can use an argument analogous to that of Sec. 7.1. For simplicity, we denote the length of the internal edges of the rescaled graph emanating from the vertex \mathcal{X}_1 by $l'_1 = l_1/c_1, \dots, l'_p = l_p/c_p$ and the weights of the corresponding internal and external edges by c_1, \dots, c_p and $\tilde{c}_1, \dots, \tilde{c}_q$, respectively. Since nothing prevents us from introducing vertices with Kirchhoff coupling condition at the distance $l_0 := \min\{l'_1, \dots, l'_p\}$ from \mathcal{X}_1 , we can employ the model sketched in Figure 3. One defines the subspace of weighted symmetric functions as

$$g_{\text{sym}1}(x) = \frac{1}{\sqrt{\sum_{j=1}^p c_j}} \sum_{j=1}^p \sqrt{c_j} g_j(x), \quad g_{\text{sym}2}(x) = \frac{1}{\sqrt{\sum_{j=1}^q \tilde{c}_j}} \sum_{j=1}^q \sqrt{\tilde{c}_j} \tilde{g}_j(x),$$

where g_j 's and \tilde{g}_j 's refer to the internal and external edges emanating from \mathcal{X}_1 , respectively. Following the argument of Section 7.1, the restriction of the Hamiltonian to this subspace can be unitarily transformed to the Hamiltonian on the segment of length l_0 and the half-line coupled mutually by the following condition

$$\frac{g_{\text{sym}1}(\mathcal{X}_1)}{\sqrt{\sum_{j=1}^p c_j}} = \frac{g_{\text{sym}2}(\mathcal{X}_1)}{\sqrt{\sum_{j=1}^q \tilde{c}_j}}, \quad \sqrt{\sum_{j=1}^p c_j} g'_{\text{sym}1}(\mathcal{X}_1) + \sqrt{\sum_{j=1}^q \tilde{c}_j} g'_{\text{sym}2}(\mathcal{X}_1) = 0$$

at \mathcal{X}_1 , where $g_{\text{sym}1}(\mathcal{X}_1)$ and $g_{\text{sym}2}(\mathcal{X}_1)$ refer to the limit of the functional values from the segment and the half-line, respectively, and $g'_{\text{sym}1}(\mathcal{X}_1)$, $g'_{\text{sym}2}(\mathcal{X}_1)$ stand for the appropriate outward derivatives. Similarly, the restriction of the Hamiltonian to the orthogonal complement of the subspace of symmetric functions leads to the Dirichlet conditions from both sides of \mathcal{X}_1 . Consequently, the effective size of the graph is less than its actual size if and only if $\sum_{j=1}^p c_j = \sum_{j=1}^q \tilde{c}_j$ at some vertex. \square

The material in this section shows that within the category of weighted graphs with appropriately generalized Kirchhoff boundary conditions, the topology of the graph has no relevance to the question of non-Weyl resonance asymptotics. After fixing the topology of the graph, one can convert it to or from the non-Weyl type by altering the weights on the leads in a suitable manner.

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